

Phosphonic acid, vinyl-, diethyl ester
682-30-4 | DTXSID70218372

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 91.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.40e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

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3-Chlorophenylurea

Measured: 102

Predicted: 57.3

Image not found

3-Bromophenylurea

Measured: 132

Predicted: 114

Image not found

(2-Chlorophenyl)urea

Measured: 40.7

Predicted: 51.3

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N-(4-Bromophenyl)urea

Measured: 115

Predicted: 122

Image not found

Acetamide, N-(3-bromophenyl)-
(9CI)

Measured: 102

Predicted: 77.2